Mathematical Modeling of Quantum Well Potentials for the Generalized Schrödinger Equations

A.A. Suzko
Laboratory of Information Technologies, JINR, Dubna

Introduction

We study intertwining relations, supersymmetry and Darboux transformations for time-dependent and time-independent generalized Schrödinger equations [3]-[8]. We obtain intertwiners in an explicit form, by means of which we construct arbitrary-order Darboux transformations for our class of equations. We develop a corresponding supersymmetric formulation and prove equivalence of the Darboux transformations with the supersymmetry formalism.

We also elaborate another method of constructing a time-dependent periodic Hamiltonian for which a system of Schrödinger equations admits analytic solutions [9]-[12]. Time-independent soluble problems are transformed into time-dependent ones by a set of unitary time-dependent transformations and a proper choice of initial states. The cyclic evolution of quantum systems for periodic in time Hamiltonians is studied. A class of periodic time-dependent Hamiltonians with cyclic solutions is constructed in a closed analytic form. The periodic time-dependent Hamiltonians are generated whose expectation values for cyclic solutions do not depend on time. It is shown, the spin-expectation values and probability density in a given point of space-time are not dependent on time, too. As a consequence, this approach can be used for modelling quantum dynamic wells and wires with the effect of a particle localization. Nonadiabatic geometric phases are calculated in terms of obtained cyclic solutions. A time-dependent periodic Hamiltonian admitting exact solutions is applied to construct a set of universal gates for quantum computer. A way of obtaining entanglement operators is discussed, too.

Reconstruction of quantum well potentials for the time-independent generalized Schrödinger equation

The study of the generalized Schrödinger equation with a position-dependent (effective) mass has recently attracted interest in condensed matter physics as well as related fields of physics. In particular, the effective mass Schrödinger equation is used for the description of electronic properties of semiconductor heterostructures and quantum dots. The concept of energy-dependent potentials is used in nuclear physics helium clusters and metal clusters. As for the semiconductor heterostructures is concerned, the progress in this area became possible, due to the development of technologies and techniques, such as *Molecular Beam Epitaxy (MBE)* for instance, which enables to deposit thin layers of different materials one on top of the other, with almost atomic precision. The last one, in its turn, provides the opportunity to produce a variety of *low-dimensional structures*. In practice the quantum wells of different shapes are produced by means of MBE technique, when the semiconductor layers are grown subsequently one by one and these layers are characterized by different electron effective masses. The subsequent semiconductor layers stuck together make the quantum well and as a result, one can consider such structure as having effective mass which depends on the space variable. One of the most important problems of quantum engineering is the construction of multi-quantum well structures possessing desirable spectral properties [1, 2]. Therefore, the problem of reconstruction of quantum well potentials with a predetermined energy spectrum is very important to extend the opportunities for investigation of low-dimensional structures. The technique of Darboux transformation operators allows the above mentioned potential reconstruction.

We construct Darboux transformations for a generalized Schrödinger equation [3]-[7]

$$-\left[\frac{d}{dx}\left(\frac{1}{m(x)}\right)\frac{d}{dx}\right]\phi(x)+v(x)\phi(x)=h(x)\mathcal{E}\phi(x)\ , \tag{1}$$

to generate the potentials which support the desirable spectrum. Here $m(x)$ stands for the particle's effective mass, $h(x)$ and $v(x)$ denote the potentials, $\phi(x)$ is the wave function and $\mathcal{E}$ denotes the real-valued energy. By using the technique of intertwining relations

$$\mathcal{L}\mathcal{H}=\mathcal{H}_1\mathcal{L}\ ,\quad \phi_1\ =\ \mathcal{L}\ \phi \tag{2}$$

we have obtained in [5] the intertwining operator $\mathcal{L}$, the transformed potential $v_1(x)$ and the corresponding solutions $\phi_1(x)$ in the form:

$$\mathcal{L}=\frac{1}{\sqrt{h\ m}}\left(\frac{d}{dx}+K\right)\ ,\qquad K=-\frac{\mathcal{U}_1{}'}{\mathcal{U}_1}, \tag{3}$$

$$v_1=v+\frac{2\sqrt{h}}{\sqrt{m}}\frac{d}{dx}\frac{K}{\sqrt{mh}}-\frac{\sqrt{h}}{\sqrt{m}}\frac{d}{dx}\left[\frac{1}{h}\frac{d}{dx}\left(\frac{\sqrt{h}}{\sqrt{m}}\right)\right] \tag{4}$$

$$\phi_1\ =\ \mathcal{L}\ \phi=\frac{1}{\sqrt{h\ m}}\left[\frac{d}{dx}-\left(\ln\mathcal{U}_1\right)'\right]\phi\ . \tag{5}$$

Note that the transformation function $\mathcal{U}_1$ define the transformation operator $\mathcal{L}$ and the new potential v_1 and corresponding solutions ϕ_1. The new potential depends not only from the potential v and from the additional potentials m and h. The method

allows one to generate isospectral potential pairs, where bound states can be added or removed in one of the partners. Our generalized Darboux transformations comprises the position-dependent effective mass case and the case of linearly energy-dependent potentials, as well as the conventional case of Schrödinger equation. Evidently, employing the Darboux transformation one more to obtained model, one can construct new exactly solvable models for the generalized Schrödinger equation.

Chain of Darboux transformations

Iterating the procedure n times in regard to the given operator $\mathcal{H}$, one arrives at the operator $\mathcal{H}_n$, which satisfies the intertwining relation

$$\mathcal{L}\mathcal{H} = \mathcal{H}_n\mathcal{L}.$$

In this way one gets [6]

$$v_n = v_{n-1} + 2\sqrt{\frac{h}{m}}\frac{d}{dx}\frac{K_n}{\sqrt{mh}} - \sqrt{\frac{h}{m}}\frac{d}{dx}\left[\frac{1}{h}\frac{d}{dx}\left(\sqrt{\frac{h}{m}}\right)\right], \quad (6)$$

$$\phi_n = \mathcal{L}\phi = \mathcal{L}_n\phi_{n-1} = \mathcal{L}_n\mathcal{L}_{n-1}...\mathcal{L}_1\phi, \quad (7)$$

where $\mathcal{L}$ is the n-th order differential operator:

$$\mathcal{L} = \mathcal{L}_n\mathcal{L}_{n-1}...\mathcal{L}_1, \quad \mathcal{L}_n = \frac{1}{\sqrt{mh}}\left(\frac{d}{dx} + K_n\right), \quad (8)$$

$$K_n = -\chi'_{n-1}\chi_{n-1}^{-1}, \qquad K_1 = -\frac{\mathcal{U}_1'}{\mathcal{U}_1}$$

and $\chi_{n-1} \equiv \chi_{n-1}(x, \lambda_n)$ is obtained by means of the "n"-order transformation, applied to the solution $\mathcal{U}_n$ of the equation (10) with the eigenvalue λ_n

$$\chi_{n-1} = \mathcal{L}_{n-1}\mathcal{U}_n = \frac{1}{\sqrt{mh}}\left(\frac{d}{dx} + K_{n-1}\right)\mathcal{U}_n. \quad (9)$$

It is clear that χ_{n-1} is the solution of (10) with the potential v_{n-1}, and χ_{n-1} can be taken as a new transformation function for the Hamiltonian $\mathcal{H}_{n-1}$ to generate a new potential. It should be noted, that the chain of n first-order Darboux transformations results in a chain of exactly solvable Hamiltonians $\mathcal{H} \to \mathcal{H}_1 \to ... \to \mathcal{H}_n$.

We have established a relation between first-order Darboux transformations, supersymmetry and factorization of the Hamiltonians that are associated with our generalized Schrödinger equation. Furthermore, our methods allow for the generation of isospectral potentials, where one of the potentials has additional or less bound states than its partner. The procedure can be repeated as many times as it is needed to construct new potential quantum well and corresponding solutions with a given spectrum. We have constructed a chain of Darboux transformations for a generalized Schrödinger equation with position dependent mass and with energy dependent potentials. On concrete examples we have shown [4]-[6] how to apply the Darboux transformations technique for modeling quantum well potentials with the given spectrum for investigation of low-dimensional structures in nanoelectronics. In the particular case of a conventional Schrödinger equation our generalized Darboux transformations reduce correctly to the well-known expressions.

Supersymmetry and Darboux transformation for the generalized time-dependent Schrödinger equation

In [7] we developed the supersymmetry formalism for generalized time-dependent Schrödinger equations with position-dependent mass and weighted energy and prove equivalence with the generalized Darboux transformation. We obtain the supersymmetric Hamiltonian with two superpartner Hamiltonians in a factorized form. Note that, instead of having factorized a scalar operator as in the conventional supersymmetry, here we have factorized a matrix operator depending on spatial and time variables. We consider the following generalized, time-dependent Schrödinger equation in $(1+1)$ dimensions and units $\hbar^2/2 = 1$:

$$i\ h\ \psi_t = -\left[\partial_x\left(\frac{1}{m}\right)\partial_x\right]\psi + v\ \psi\ , \quad (10)$$

where the index and the symbol ∂ denote partial differentiation, $m = m(x,t)$ stands for the particle's effective mass, $h = h(x,t)$ and $v = v(x,t)$ denote the potentials, and $\psi = \psi(x,t)$ is the solution. By using the intertwining operator technique

$$\mathcal{L}(i\partial_t - \mathcal{H}) = (i\partial_t - \widetilde{\mathcal{H}})\mathcal{L}\ , \quad \widetilde{\phi}\ =\ \mathcal{L}\ \phi \quad (11)$$

we obtain the explicit form of the transformed potential $\widetilde{v}$, the intertwiner $\mathcal{L}$ and the transformed solution $\widetilde{\psi}$, respectively:

$$\widetilde{v} = v\ -\ 2\sqrt{\frac{h}{m}}\left[\frac{(u_1)_x}{u_1\sqrt{hm}}\right]_x - \sqrt{\frac{h}{m}}\left[\frac{1}{h}\left(\sqrt{\frac{h}{m}}\right)_x\right]_x + ih\left[\frac{\beta_t}{\beta} - \frac{1}{2}\ \log(hm)_t\right], \quad (12)$$

$$\mathcal{L} = \frac{\beta}{\sqrt{h\ m}}\left(\partial_x + K\right) = \frac{\beta}{\sqrt{h\ m}}\left[\partial_x - \log(\mathcal{U})_x\right] \quad (13)$$

$$\tilde{\psi} = \mathcal{L}\psi = \frac{\beta}{\sqrt{h\ m}}\left[\partial_x - \log(\mathcal{U})_x\right]\psi, \quad (14)$$

where $\beta = \beta(t)$ is an arbitrary, purely time-dependent constant of integration. The transformation function $\mathcal{U}$ defines the transformation operator $\mathcal{L}$, the new potential $\tilde{v}$ and corresponding solutions $\tilde{\psi}$. It was shown in [7] that the initial Hamiltonian $\mathcal{H}$ and the transformed Hamiltonian $\widetilde{\mathcal{H}}$ can be factorized

$$\mathcal{H} = \mathcal{L}^{+}\mathcal{L} + \lambda_1 \ , \qquad (15)$$

$$\widetilde{\mathcal{H}} = \mathcal{L}\,\mathcal{L}^{+} + \lambda_2, \qquad (16)$$

or in an equivalent form

$$H_m = \left\{Q^{+}, Q\right\} + \Lambda. \qquad (17)$$

Here Λ is a diagonal factorization matrix $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2)$ with elements $\lambda_1 = \lambda_1(x,t)$ and $\lambda_2 = \lambda_2(x,t)$ depending on spatial and time variables. It is shown that

$$\lambda_1 = i\,\frac{\mathcal{U}_t}{\mathcal{U}} - C \ , \qquad \lambda_2 = \lambda_1 + i\,\frac{B_t}{B} - C \ ,$$

where C is an integration constant and $B = \beta/\sqrt{h\ m}$.

The fact that the factorization matrix Λ depends on spatial and time variables through the functions $\mathcal{U} = \mathcal{U}(x,t)$ and $B = B(x,t)$ is *nonstandard*. In a particular case, when the potentials m and h do not depend on time, Λ can be written as $\Lambda = \lambda_1 I$, where I is the identity matrix. Moreover, if the transformation function $\mathcal{U}$ can be presented in a factorized form like $\mathcal{U}(x,t) = F(x)S(t)$, then λ_1 becomes independent of the spatial variable.

We have studied in [7, 8] intertwining relations, supersymmetry and Darboux transformations for time-dependent generalized Schrödinger equations. We have obtained intertwiners in an explicit form, by means of which we construct arbitrary-order Darboux transformations for our class of equations. We developed a corresponding supersymmetric formulation and proved equivalence of the Darboux transformations with the supersymmetry formalism. Finally we have shown that our Darboux transformations can also be constructed by means of point transformations, avoiding the use of intertwiners.

Periodic time-dependent Hamiltonians

In the papers [9]-[12] we elaborated a technique of constructing a periodic time-dependent Hamiltonian admitting exact solutions with the use of an exactly soluble time-independent Hamiltonian, unitary time-dependent transformations and a proper choice of initial states. A class of periodic time-dependent Hamiltonians with cyclic solutions is constructed in a closed analytic form. In particular, the periodic time-dependent Hamiltonians are generated whose expectation values for cyclic solutions and spin-expectation values do not depend on time. It means that time-dependent equations for the obtained time-periodic potentials possess solutions and properties like time-independent ones. As a consequence, this approach can be used for modeling quantum dynamic wells with properties of dynamic localization. The time evolution matrices are obtained in an explicit form and used to construct logic gates for computation [10]-[12]. A way of obtaining entanglement operator is discussed, too.

Recent achievements in microfabrication technology afford opportunities of constructing two-dimensional quantum wells, superlattices, quantum wires and dots with properties of particle confinement. As it was shown in [W. Paul and M. Raether, Z.Phys. vol. 140, (1955) 262] and [A.V. Gaponov and M.A. Miller, J.Eksper.Teor.Fiz.], under definite conditions a particle can be localized in a nonuniform high frequency electromagnetic field. Paul and Raether, Gaponov and Miller considered the classical movement. Quantum mechanical analysis has been made in [I.E. Tralle, Phys.Stat.Sol. 1994, vol.181, p.97; R. Cook et.al., Phys.Rev., 1985, vol. A31, p.564, V.N. Gheorghe and F. Vedel, Phys. Rev., 1992, vol. A45, p.4828]. They considered a particle motion in a rapidly oscillating field of the form $V(r,t) = V(r)\cos\omega t$ in terms of the Shcrödinger equations with periodic $V(r)$. Their main result is that for a sufficiently high frequency ω the time-dependent potential is equivalent to the time-independent effective potential and, as a sequence, a particle can be confined. This result is a quantum-mechanical analog of the Gaponov, Miller, Paul effect. We generated more complicated time-dependent potentials which with special initial functions give the effect like time-independent potentials and can be used for investigation of the dynamic particle localization.

Suggested method allows to generate exactly soluble time-dependent Hamiltonians from time-independent ones. The time evolution matrices are obtained in an explicit form and used to construct logic gates for computation. The approach opens opportunities for modeling quantum dynamic systems with predetermined properties, in particular, quantum wells with properties of dynamic localization.

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